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Ab initio and DFT Calculation of Conformational Properties and Thermodynamic Properties of Sterically Congested 5-(4-Bromophenyl)-N-(trichloroacetyl)-1,3,4-oxadiazole-2-carboxamide

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Introduction

In the past decade, IR spectroscopy have become important techniques for obtaining information on chemical structures and are applied in virtually all branches of chemistry. Vibrational spectroscopy is used extensively in organic chemistry for the identification of functional groups of organic compounds as well as for studies on molecular conformation, reaction kinetics, etc [1]. Density functional theory (DFT) has become a major tool in the methodological arsenal of computational organic chemists. DFT methods are increasingly applied to representative pharmacological compounds aiming to elucidate their molecular structures, electronic properties and bonds, the establishment of electronic and structural factors of selected reactions and their mechanisms. Experimental measurements and theoretical calculations on vibrational frequencies become one of the key factors in the molecular structure correlations design. For a proper understanding of IR and Raman spectra, a reliable assignment of all vibrational bands is essential. For this purpose, the quantum chemical methods, ranging from semi-empirical to DFT approaches, are invaluable tools [2,3], On the other hand, DFT methods, particularly hybrid functional methods, have evolved to a powerful quantum chemical tool for the determination of the electronic structure of molecules. Among these, the B3LYP combination is the most used since it proved its ability in reproducing various molecular properties, including vibrational spectra. In connection with our recent interest to multicomponent reactions, we report synthesis and FT-IR studies of 5-(4-Bromophenyl)-N-(trichloroacetyl)-1,3,4-oxadiazole-2-carboxamide. The B3LYP/HF calculations for computation of FT-IR spectra have been carried out for the title compounds at the 6-31G* and 6-311++G** basis set levels. Predicted vibrational frequencies have been assigned and compared with experimental FT-IR spectra and they are supported each other.



Computational details

The vibrational wavenumbers were calculated using the Gaussian 98 software package on a Pentium IV personal computer. Geometry optimizations were performed with B3LYP/6-31G* , B3LYP/6-311++G**, and HF/6-311++G** methods. The DFT technique employed the Becke3 (B3) (Becke 1992) exchange functional which supplement with Lee, Yang, Parr (LYP) (Lee et al., 1988) correlation functional

Results and Discussion

The reaction proceeds smoothly and cleanly under mild conditions and no side reactions are observed. The structures of the products were deduced from their IR, ¹H NMR, ¹³C NMR and elemental analyses. In the present study, we report the B3LYP/HF calculation results for sterically congested 5-(4-Bromophenyl)-N -(trichloroacetyl)-1,3,4-oxadiazole-2-carboxamide in order to give their optimal molecular geometry and vibrational modes. Here, we focus on the use of modern density functional theory to fully account for the experimental vibrational IR data for the products. In the literature, any theoretical vibrational studies on the title compounds were not found. The schematic drawing with the theoretical geometric structure is shown in this paper.

The observed FT-IR bands and calculated wavenumbers and assignments are given. On the basis of our calculations and experimental infrared spectra, we made a reliable one-to-one correspondence between our fundamentals and any of our wavenumbers calculated by B3LYP and HF methods. For the title compound the strong band at 3393 in the FT-IR spectrum is assigned as ν_{NH} mode. The calculated value for this mode are 3399, 3406, 3390, and 3395 cm^{-1} for HF/6-311++G**, B3LYP/6-31G*, and B3LYP/6-311++G** levels, respectively. The carbonyl stretching C=O vibration of ketone for compound appears at 1699. The calculated value for this mode are 11715, 1719, 1721, and 1698 cm^{-1} for HF/6-31G*, HF/6-311++G**, B3LYP/6-31G*, and B3LYP/6-311++G** levels, respectively.

The overall agreement between theory and experiment is quite reasonable for all methods that we have used. We further found a reliable one-to-one correspondence between our fundamentals and any of our calculated frequencies. There is an excellent agreement between experimental and theoretical results. In order to compare of this agreement, the correlation graphic based on the theoretical and experimental data has been investigated.



References

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